Rino Ragno

List of Publications by Year
in descending order

145 papers	4,791 citations	76196 40 h-index	123241 61 g-index
148 all docs	148 docs citations	148 times ranked	6135 citing authors

#	Article	IF	Citations
1	Histone deacetylation in epigenetics: An attractive target for anticancer therapy. Medicinal Research Reviews, 2005, 25, 261-309.	5.0	306
2	Lycium barbarum polysaccharides: Extraction, purification, structural characterisation and evidence about hypoglycaemic and hypolipidaemic effects. A review. Food Chemistry, 2018, 254, 377-389.	4.2	192
3	Design, Synthesis, and Biological Evaluation of Sirtinol Analogues as Class III Histone/Protein Deacetylase (Sirtuin) Inhibitors. Journal of Medicinal Chemistry, 2005, 48, 7789-7795.	2.9	159
4	Design, Molecular Modeling, Synthesis, and Anti-HIV-1 Activity of New Indolyl Aryl Sulfones. Novel Derivatives of the Indole-2-carboxamide. Journal of Medicinal Chemistry, 2006, 49, 3172-3184.	2.9	157
5	Antimycobacterial pyrroles: synthesis, anti- Mycobacterium tuberculosis activity and QSAR studies. Bioorganic and Medicinal Chemistry, 2000, 8, 1423-1432.	1.4	129
6	3-(4-Aroyl-1-methyl-1H-2-pyrrolyl)-N-hydroxy-2-alkylamides as a New Class of Synthetic Histone Deacetylase Inhibitors. 1. Design, Synthesis, Biological Evaluation, and Binding Mode Studies Performed through Three Different Docking Procedures. Journal of Medicinal Chemistry, 2003, 46, 512-524.	2.9	113
7	Small Molecule Inhibitors of Histone Arginine Methyltransferases:â€‰ Homology Modeling, Molecular Docking, Binding Mode Analysis, and Biological Evaluations. Journal of Medicinal Chemistry, 2007, 50, 1241-1253.	2.9	98
8	Computer-Aided Design, Synthesis, and Anti-HIV-1 Activity in Vitro of 2-Alkylamino-6-[1-(2,6-difluorophenyl)alkyl]-3,4-dihydro-5-alkylpyrimidin-4(3H)- ones as Novel Potent Non-Nucleoside Reverse Transcriptase Inhibitors, Also Active Against the Y181C Variant. Journal of Medicinal Chemistry, 2004, 47, 928-934.	2.9	85
9	Structure-Based Design, Synthesis, and Biological Evaluation of Conformationally Restricted Novel 2-Alkylthio-6-[1-(2,6-difluorophenyl)alkyl]- 3,4-dihydro-5-alkylpyrimidin-4(3H)-ones as Non-nucleoside Inhibitors of HIV-1 Reverse Transcriptase. Journal of Medicinal Chemistry, 2001, 44, 2544-2554.	2.9	84
10	3-(4-Aroyl-1H-pyrrol-2-yl)-N-hydroxy-2-propenamides, a New Class of Synthetic Histone Deacetylase Inhibitors. Journal of Medicinal Chemistry, 2001, 44, 2069-2072.	2.9	79
11	Docking and 3-D QSAR Studies on Indolyl Aryl Sulfones. Binding Mode Exploration at the HIV-1 Reverse Transcriptase Non-Nucleoside Binding Site and Design of Highly ActiveN-(2-Hydroxyethyl)carboxamide andN-(2-Hydroxyethyl)carbohydrazide Derivatives. Journal of Medicinal Chemistry, 2005, 48, 213-223.	2.9	77
12	2,6-Bis(3,4,5-trihydroxybenzylydene) derivatives of cyclohexanone. Bioorganic and Medicinal Chemistry, 2004, 12, 199-215.	1.4	76
13	HIV-Reverse Transcriptase Inhibition:â€‰ Inclusion of Ligand-Induced Fit by Cross-Docking Studies. Journal of Medicinal Chemistry, 2005, 48, 200-212.	2.9	67
14	Binding Mode Analysis of 3-(4-Benzoyl-1-methyl-1H-2-pyrrolyl)-N-hydroxy-2-propenamide:Â A New Synthetic Histone Deacetylase Inhibitor Inducing Histone Hyperacetylation, Growth Inhibition, and Terminal Cell Differentiation. Journal of Medicinal Chemistry, 2002, 45, 1778-1784.	2.9	65
15	Synthesis, Biological Evaluation, and Binding Mode of Novel 1-[2-(Diarylmethoxy)ethyl]-2-methyl-5-nitroimidazoles Targeted at the HIV-1 Reverse Transcriptase. Journal of Medicinal Chemistry, 2002, 45, 1567-1576.	2.9	65
16	3-(4-Aroyl-1-methyl-1H-pyrrol-2-yl)-N-hydroxy-2-propenamides as a New Class of Synthetic Histone Deacetylase Inhibitors. 3. Discovery of Novel Lead Compounds through Structure-Based Drug Design and Docking Studiesâ€Ì”. Journal of Medicinal Chemistry, 2004, 47, 1351-1359.	2.9	65
17	Mentha suaveolens Ehrh. (Lamiaceae) Essential Oil and Its Main Constituent Piperitenone Oxide: Biological Activities and Chemistry. Molecules, 2015, 20, 8605-8633.	1.7	65
18	In vitro inhibition of herpes simplex virus type 1 replication by Mentha suaveolens essential oil and its main component piperitenone oxide. Phytomedicine, 2014, 21, 857-865.	2.3	63

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19	High Potency of Melaleuca alternifolia Essential Oil against Multi-Drug Resistant Gram-Negative Bacteria and Methicillin-Resistant Staphylococcus aureus. Molecules, 2018, 23, 2584.	1.7	62
20	Antimicrobial and Antibiofilm Activity and Machine Learning Classification Analysis of Essential Oils from Different Mediterranean Plants against Pseudomonas aeruginosa. Molecules, 2018, 23, 482.	1.7	62
21	3-(4-Aroyl-1-methyl-1H-2-pyrrolyl)-N-hydroxy-2-propenamides as a New Class of Synthetic Histone Deacetylase Inhibitors. 2. Effect of Pyrrole-C2and/or -C4Substitutions on Biological Activityâ€. Journal of Medicinal Chemistry, 2004, 47, 1098-1109.	2.9	61
22	Calamintha nepeta (L.) Savi and its Main Essential Oil Constituent Pulegone: Biological Activities and Chemistry. Molecules, 2017, 22, 290.	1.7	61
23	Design, Synthesis and Biological Evaluation of Carboxy Analogues of Arginine Methyltransferase Inhibitorâ€...1 (AMIâ€1). ChemMedChem, 2010, 5, 398-414.	1.6	60
24	Molecular Modeling of Azole Antifungal Agents Active againstCandida albicans. 1. A Comparative Molecular Field Analysis Study1. Journal of Medicinal Chemistry, 1996, 39, 1227-1235.	2.9	59
25	Synthesis and Biological Properties of Novel, Uracil-Containing Histone Deacetylase Inhibitors. Journal of Medicinal Chemistry, 2006, 49, 6046-6056.	2.9	57
26	Esential oils extraction: a 24-hour steam distillation systematic methodology. Natural Product Research, 2017, 31, 2387-2396.	1.0	56
27	Synthesis and Biological Properties of Novel 2-Aminopyrimidin-4(3H)-ones Highly Potent against HIV-1 Mutant Strains. Journal of Medicinal Chemistry, 2007, 50, 5412-5424.	2.9	55
28	Combining 3-D Quantitative Structureâ^'Activity Relationship with Ligand Based and Structure Based Alignment Procedures for in Silico Screening of New Hepatitis C Virus NS5B Polymerase Inhibitors. Journal of Chemical Information and Modeling, 2010, 50, 662-676.	2.5	54
29	Synthesis and Biological Validation of Novel Synthetic Histone/Protein Methyltransferase Inhibitors. ChemMedChem, 2007, 2, 987-991.	1.6	52
30	5-Alkyl-6-benzyl-2-(2-oxo-2-phenylethylsulfanyl)pyrimidin-4(3H)-ones, a Series of Anti-HIV-1 Agents of the Dihydro-alkoxy-benzyl-oxopyrimidine Family with Peculiar Structureâ^'Activity Relationship Profile. Journal of Medicinal Chemistry, 2008, 51, 4641-4652.	2.9	52
31	Novel 1-[2-(Diarylmethoxy)ethyl]-2-methyl-5-nitroimidazoles as HIV-1 Non-Nucleoside Reverse Transcriptase Inhibitors. A Structureâ^'Activity Relationship Investigation. Journal of Medicinal Chemistry, 2005, 48, 4378-4388.	2.9	51
32	Carotenoid content of Goji berries: CIELAB, HPLC-DAD analyses and quantitative correlation. Food Chemistry, 2018, 268, 49-56.	4.2	49
33	Beneficial effect of Mentha suaveolens essential oil in the treatment of vaginal candidiasis assessed by real-time monitoring of infection. BMC Complementary and Alternative Medicine, 2011, 11, 18.	3.7	47
34	5-Alkyl-2-alkylamino-6-(2,6-difluorophenylalkyl)-3,4-dihydropyrimidin-4(3H)-ones, a new series of potent, broad-spectrum non-nucleoside reverse transcriptase inhibitors belonging to the DABO family. Bioorganic and Medicinal Chemistry, 2005, 13, 2065-2077.	1.4	46
35	Design, synthesis and biological evaluation of new classes of thieno[3,2-d]pyrimidinone and thieno[1,2,3]triazine as inhibitor of vascular endothelial growth factor receptor-2 (VEGFR-2). European Journal of Medicinal Chemistry, 2013, 63, 765-781.	2.6	46
36	3-D QSAR Studies on Histone Deacetylase Inhibitors. A GOLPE/GRID Approach on Different Series of Compounds. Journal of Chemical Information and Modeling, 2006, 46, 1420-1430.	2.5	42

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37	The Tumor Marker Human Placental Protein 11 Is an Endoribonuclease. Journal of Biological Chemistry, 2008, 283, 34712-34719.	1.6	42
38	Effects ofMentha suaveolensEssential Oil Alone or in Combination with Other Drugs inCandida albicans. Evidence-based Complementary and Alternative Medicine, 2014, 2014, 1-9.	0.5	41
39	Machine Learning Analyses on Data including Essential Oil Chemical Composition and In Vitro Experimental Antibiofilm Activities against Staphylococcus Species. Molecules, 2019, 24, 890.	1.7	41
40	RIP1â€“HAT1â€“SIRT Complex Identification and Targeting in Treatment and Prevention of Cancer. Clinical Cancer Research, 2018, 24, 2886-2900.	3.2	40
41	Class II-selective histone deacetylase inhibitors. Part 2: Alignment-independent GRIND 3-D QSAR, homology and docking studies. European Journal of Medicinal Chemistry, 2008, 43, 621-632.	2.6	39
42	Design, synthesis and QSAR studies on N-aryl heteroarylisopropanolamines, a new class of non-peptidic HIV-1 protease inhibitors. Bioorganic and Medicinal Chemistry, 2002, 10, 2511-2526.	1.4	38
43	www.3d-qsar.com: a web portal that brings 3-D QSAR to all electronic devicesâ€"the Py-CoMFA web application as tool to build models from pre-aligned datasets. Journal of Computer-Aided Molecular Design, 2019, 33, 855-864.	1.3	37
44	The Targeted Pesticides as Acetylcholinesterase Inhibitors: Comprehensive Cross-Organism Molecular Modelling Studies Performed to Anticipate the Pharmacology of Harmfulness to Humans In Vitro. Molecules, 2018, 23, 2192.	1.7	36
45	Identification of glutathione-methacrylates adducts in gingival fibroblasts and erythrocytes by HPLCâ€“MS and capillary electrophoresis. Dental Materials, 2011, 27, e87-e98.	1.6	35
46	New Inhibitors of Indoleamine 2,3-Dioxygenase 1: Molecular Modeling Studies, Synthesis, and Biological Evaluation. Journal of Medicinal Chemistry, 2016, 59, 9760-9773.	2.9	35
47	Design, synthesis and biological evaluation of heteroaryl diketohexenoic and diketobutanoic acids as HIV-1 integrase inhibitors endowed with antiretroviral activity. Il Farmaco, 2005, 60, 409-417.	0.9	34
48	Essential oil extraction, chemical analysis and anti-Candida activity of Foeniculum vulgare Miller â€“ new approaches. Natural Product Research, 2018, 32, 1254-1259.	1.0	34
49	3-D QSAutogrid/R: An Alternative Procedure To Build 3-D QSAR Models. Methodologies and Applications. Journal of Chemical Information and Modeling, 2012, 52, 1674-1685.	2.5	33
50	Multidisciplinary Approach to Determine the Optimal Time and Period for Extracting the Essential Oil from Mentha suaveolens Ehrh. Molecules, 2015, 20, 9640-9655.	1.7	33
51	Understanding the Molecular Determinant of Reversible Human Monoamine Oxidase B Inhibitors Containing 2H-Chromen-2-One Core: Structure-Based and Ligand-Based Derived Three-Dimensional Quantitative Structureâ€“Activity Relationships Predictive Models. Journal of Chemical Information and Modeling, 2017, 57, 787-814.	2.5	33
52	6-Aryl-2,4-dioxo-5-hexenoic acids, novel integrase inhibitors active against HIV-1 multiplication in cell-based assays. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 1745-1749.	1.0	32
53	Antimicrobial Essential Oil Formulation: Chitosan Coated Nanoemulsions for Nose to Brain Delivery. Pharmaceutics, 2020, 12, 678.	2.0	32
54	Essential Oil Extraction, Chemical Analysis and Anti-Candida Activity of Calamintha nepeta (L.) Savi subsp. glandulosa (Req.) Ballâ€"New Approaches. Molecules, 2017, 22, 203.	1.7	30

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55	Essential oils against bacterial isolates from cystic fibrosis patients by means of antimicrobial and unsupervised machine learning approaches. Scientific Reports, 2020, 10, 2653.	1.6	30
56	2-(Alkyl/Aryl)Amino-6-Benzylpyrimidin-4(3H)-ones as Inhibitors of Wild-Type and Mutant HIV-1: Enantioselectivity Studies. Journal of Medicinal Chemistry, 2012, 55, 3558-3562.	2.9	29
57	Shmt2: A Stat3 Signaling New Player in Prostate Cancer Energy Metabolism. Cells, 2019, 8, 1048.	1.8	28
58	Hsp90 Inhibitors, Part 2: Combining Ligand-Based and Structure-Based Approaches for Virtual Screening Application. Journal of Chemical Information and Modeling, 2014, 54, 970-977.	2.5	27
59	Exploring the first Rimonabant analog-opioid peptide hybrid compound, as bivalent ligand for CB1 and opioid receptors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2017, 32, 444-451.	2.5	27
60	Chemical composition and antimicrobial activity of essential oil of Helichrysum italicum (Roth) G. Don fil. (Asteraceae) from Montenegro. Natural Product Research, 2020, 34, 445-448.	1.0	27
61	Teaching and Learning Computational Drug Design: Student Investigations of 3D Quantitative Structureâ€“Activity Relationships through Web Applications. Journal of Chemical Education, 2020, 97, 1922-1930.	1.1	27
62	Chiral resolution and molecular modeling investigation ofrac-2-cyclopentylthio-6-[1-(2,6-difluorophenyl)ethyl]-3,4-dihydro-5-methylpyrimidin-4(3H)-one (MC-1047), a potent anti-HIV-1 reverse transcriptase agent of the DABO class. Chirality, 2001, 13, 75-80.	1.3	26
63	Histone Deacetylase Inhibitors: Structure-Based Modeling and Isoform-Selectivity Prediction. Journal of Chemical Information and Modeling, 2012, 52, 2215-2235.	2.5	26
64	Indolyl Aryl Sulphones as HIV-1 Non-Nucleoside Reverse Transcriptase Inhibitors: Synthesis, Biological Evaluation and Binding Mode Studies of New Derivatives at Indole-2-carboxamide. Antiviral Chemistry and Chemotherapy, 2006, 17, 59-77.	0.3	25
65	New pyrrole-based histone deacetylase inhibitors: Binding mode, enzyme- and cell-based investigations. International Journal of Biochemistry and Cell Biology, 2009, 41, 235-247.	1.2	24
66	Novel coumarin- and quinolinone-based polycycles as cell division cycle 25-A and -C phosphatases inhibitors induce proliferation arrest and apoptosis in cancer cells. European Journal of Medicinal Chemistry, 2017, 134, 316-333.	2.6	24
67	Antitumor effect of Melaleuca alternifolia essential oil and its main component terpinen-4-ol in combination with target therapy in melanoma models. Cell Death Discovery, 2021, 7, 127.	2.0	24
68	Synthesis and evaluation of new tripeptide phosphonate inhibitors of MMP-8 and MMP-2. European Journal of Medicinal Chemistry, 2005, 40, 271-279.	2.6	23
69	CYP19 (aromatase): Exploring the scaffold flexibility for novel selective inhibitors. Bioorganic and Medicinal Chemistry, 2008, 16, 8349-8358.	1.4	23
70	Chemically Modified Multiwalled Carbon Nanotubes Electrodes with Ferrocene Derivatives through Reactive Landing. Journal of Physical Chemistry C, 2011, 115, 4863-4871.	1.5	23
71	Effects ofMentha suaveolensEssential Oil onChlamydia trachomatis. BioMed Research International, 2015, 2015, 1-7.	0.9	23
72	Chemical and Antimicrobial Analyses of Sideritis romana L. subsp. purpurea (Tal. ex Benth.) Heywood, an Endemic of the Western Balkan. Molecules, 2017, 22, 1395.	1.7	22

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73	Synthesis, biological evaluation and docking analysis of a new series of methylsulfonyl and sulfamoyl acetamides and ethyl acetates as potent COX-2 inhibitors. Bioorganic and Medicinal Chemistry, 2015, 23, 810-820.	1.4	21
74	Synthesis, biological evaluation and quantitative structure-active relationships of 1,3-thiazolidin-4-one derivatives. A promising chemical scaffold endowed with high antifungal potency and low cytotoxicity. European Journal of Medicinal Chemistry, 2017, 140, 274-292.	2.6	21
75	Synthesis and biological evaluation of enantiomerically pure pyrrolyl-oxazolidinones as a new class of potent and selective monoamine oxidase type A inhibitors. Il Farmaco, 2003, 58, 231-241.	0.9	20
76	Aroyl-Pyrrolyl Hydroxyamides: Influence of Pyrrole C4-Phenylacetyl Substitution on Histone Deacetylase Inhibition. ChemMedChem, 2006, 1, 225-237.	1.6	20
77	Inhibition of hepatitis C virus NS5B polymerase by S-trityl-l-cysteine derivatives. European Journal of Medicinal Chemistry, 2012, 49, 191-199.	2.6	20
78	Decreasing acidity in a series of aldose reductase inhibitors: 2-Fluoro-4-(1H-pyrrol-1-yl)phenol as a scaffold for improved membrane permeation. Bioorganic and Medicinal Chemistry, 2014, 22, 2194-2207.	1.4	20
79	High Potency of Indolyl Aryl Sulfone Nonnucleoside Inhibitors towards Drug-Resistant Human Immunodeficiency Virus Type 1 Reverse Transcriptase Mutants Is Due to Selective Targeting of Different Mechanistic Forms of the Enzyme. Antimicrobial Agents and Chemotherapy, 2005, 49, 4546-4554.	1.4	19
80	Design, Synthesis, Biological Evaluation, and Molecular Modeling Studies of TIBO-Like Cyclic Sulfones as Non-Nucleoside HIV-1 Reverse Transcriptase Inhibitors. ChemMedChem, 2006, 1, 82-95.	1.6	19
81	Essential Oils and Their Main Chemical Components: The Past 20 Years of Preclinical Studies in Melanoma. Cancers, 2020, 12, 2650.	1.7	19
82	Experimental Data Based Machine Learning Classification Models with Predictive Ability to Select in Vitro Active Antiviral and Non-Toxic Essential Oils. Molecules, 2020, 25, 2452.	1.7	19
83	Novel Cinnamyl Hydroxyamides and 2â€Aminoanilides as Histone Deacetylase Inhibitors: Apoptotic Induction and Cytodifferentiation Activity. ChemMedChem, 2011, 6, 698-712.	1.6	17
84	Biaryl tetrazolyl ureas as inhibitors of endocannabinoid metabolism: Modulation at the N-portion and distal phenyl ring. European Journal of Medicinal Chemistry, 2013, 63, 118-132.	2.6	17
85	Exploring the Role of 2-Chloro-6-fluoro Substitution in 2-Alkylthio-6-benzyl-5-alkylpyrimidin-4(3H)-ones: Effects in HIV-1-Infected Cells and in HIV-1 Reverse Transcriptase Enzymes. Journal of Medicinal Chemistry, 2014, 57, 5212-5225.	2.9	17
86	Melissa officinalis L. subsp. altissima (Sibth. & Sm.) Arcang. essential oil: Chemical composition and preliminary antimicrobial investigation of samples obtained at different harvesting periods and by fractionated extractions. Industrial Crops and Products, 2018, 117, 317-321.	2.5	17
87	Essential Oils Biofilm Modulation Activity, Chemical and Machine Learning Analysisâ€”Application on Staphylococcus aureus Isolates from Cystic Fibrosis Patients. International Journal of Molecular Sciences, 2020, 21, 9258.	1.8	17
88	Genotoxicity assessment of piperitenone oxide: An inÂvitro and in silico evaluation. Food and Chemical Toxicology, 2017, 106, 506-513.	1.8	16
89	Altered mitochondrial function in cells carrying a premutation or unmethylated full mutation of the FMR1 gene. Human Genetics, 2020, 139, 227-245.	1.8	16
90	The antiâ€STAT1 polyphenol myricetin inhibits M1 microglia activation and counteracts neuronal death. FEBS Journal, 2021, 288, 2347-2359.	2.2	16

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91	Comprehensive model of wild-type and mutant HIV-1 reverse transciptases. Journal of Computer-Aided Molecular Design, 2012, 26, 907-919.	1.3	15
92	Disruptor of telomeric silencing 1-like (DOT1L): disclosing a new class of non-nucleoside inhibitors by means of ligand-based and structure-based approaches. Journal of Computer-Aided Molecular Design, 2018, 32, 435-458.	1.3	15
93	Development of alkyl glycerone phosphate synthase inhibitors: Structure-activity relationship and effects on ether lipids and epithelial-mesenchymal transition in cancer cells. European Journal of Medicinal Chemistry, 2019, 163, 722-735.	2.6	15
94	In vivo Antiphytoviral Activity of Essential Oils and Hydrosols From Origanum vulgare, Thymus vulgaris, and Rosmarinus officinalis to Control Zucchini Yellow Mosaic Virus and Tomato Leaf Curl New Delhi Virus in Cucurbita pepo L.. Frontiers in Microbiology, 2022, 13, 840893.	1.5	15
95	Effect of Î±-Methoxy Substitution on the Anti-HIV Activity of Dihydropyrimidin-4(3H)-ones. Journal of Medicinal Chemistry, 2019, 62, 604-621.	2.9	14
96	Investigation on QSAR and binding mode of a new class of human rhinovirus-14 inhibitors by CoMFA and docking experiments. Bioorganic and Medicinal Chemistry, 1996, 4, 1715-1724.	1.4	13
97	Enhancing activity and selectivity in a series of pyrrol-1-yl-1-hydroxypyrazole-based aldose reductase inhibitors: The case of trifluoroacetylation. European Journal of Medicinal Chemistry, 2017, 130, 328-335.	2.6	13
98	Hsp90 Inhibitors, Part 1: Definition of 3-D QSAutogrid/R Models as a Tool for Virtual Screening. Journal of Chemical Information and Modeling, 2014, 54, 956-969.	2.5	12
99	In-Vitro Evaluation of Different Antimicrobial Combinations with and without Colistin Against Carbapenem-Resistant Acinetobacter Baumannii. Molecules, 2019, 24, 886.	1.7	12
100	Potent In Vitro Activity of Citrus aurantium Essential Oil and Vitis vinifera Hydrolate Against Gut Yeast Isolates from Irritable Bowel Syndrome Patientsâ€"The Right Mix for Potential Therapeutic Use. Nutrients, 2020, 12, 1329.	1.7	12
101	Transcriptomic and genomic studies classify NKL54 as a histone deacetylase inhibitor with indirect influence on MEF2-dependent transcription. Nucleic Acids Research, 2022, 50, 2566-2586.	6.5	12
102	Targeting the anti-apoptotic Bcl-2 family proteins: machine learning virtual screening and biological evaluation of new small molecules. Theranostics, 2022, 12, 2427-2444.	4.6	12
103	A Combination of Molecular Dynamics and Docking Calculations to Explore the Binding Mode of ADS-J1, a Polyanionic Compound Endowed with Anti-HIV-1 Activity. Journal of Chemical Information and Modeling, 2006, 46, 1344-1351.	2.5	11
104	Antibacterial activity of essential oils mixture against PSA. Natural Product Research, 2016, 30, 412-418.	1.0	11
105	Ab-initio and experimental study of pentose sugar dehydration mechanism in the gas phase. Carbohydrate Research, 2018, 458-459, 19-28.	1.1	11
106	Essential Oils Biofilm Modulation Activity and Machine Learning Analysis on Pseudomonas aeruginosa Isolates from Cystic Fibrosis Patients. Microorganisms, 2022, 10, 887.	1.6	11
107	Anti-Virulence Properties of Coridothymus capitatus Essential Oil against Pseudomonas aeruginosa Clinical Isolates from Cystic Fibrosis Patients. Microorganisms, 2021, 9, 2257.	1.6	10
108	Pharmacophore Assessment Through 3-D QSAR: Evaluation of the Predictive Ability on New Derivatives by the Application on a Series of Antitubercular Agents. Journal of Chemical Information and Modeling, 2013, 53, 1463-1474.	2.5	9

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109	Vascular endothelial growth factor receptor-2 (VEGFR-2) inhibitors: development and validation of predictive 3-D QSAR models through extensive ligand- and structure-based approaches. Journal of Computer-Aided Molecular Design, 2015, 29, 757-776.	1.3	9
110	Sideritis romana L. subsp. purpurea (Tal. ex Benth.) Heywood, a new chemotype from Montenegro. Natural Product Research, 2018, 32, 1056-1061.	1.0	9
111	Small-Molecule Interferon Inducers. Toward the Comprehension of the Molecular Determinants through Ligand-Based Approaches. Journal of Chemical Information and Modeling, 2009, 49, 1777-1786.	2.5	8
112	Identification of Smallâ€Molecule Inhibitors of the XendoU Endoribonucleases Family. ChemMedChem, 2011, 6, 1797-1805.	1.6	8
113	Breakthroughs in Medicinal Chemistry: New Targets and Mechanisms, New Drugs, New Hopesâ€“6. Molecules, 2020, 25, 119.	1.7	8
114	Identification of Inhibitors to Trypanosoma cruzi Sirtuins Based on Compounds Developed to Human Enzymes. International Journal of Molecular Sciences, 2020, 21, 3659.	1.8	8
115	Binding of azole drugs to heme: A combined MS/MS and computational approach. Polyhedron, 2015, 90, 245-251.	1.0	7
116	First-in-Class Inhibitors of the Ribosomal Oxygenase MINA53. Journal of Medicinal Chemistry, 2021, 64, 17031-17050.	2.9	7
117	Antifungal Agents, II: Synthesis and Antifungal Activities of Aryl-1H-pyrrol-2-yl-1H-imidazol-1-yl-methane Derivatives with Unsaturated Chains. Archiv Der Pharmazie, 1993, 326, 539-546.	2.1	6
118	[[[(Thienylcarbonyl)alkyl]oxy]phenyl]- and [[[(Pyrrylcarbonyl)alkyl]oxy]phenyl]oxazoline Derivatives with Potent and Selective Antihuman Rhinovirus Activity. Journal of Medicinal Chemistry, 1995, 38, 803-809.	2.9	6
119	A Series of COXâ€2 Inhibitors Endowed with NOâ€Releasing Properties: Synthesis, Biological Evaluation, and Docking Analysis. ChemMedChem, 2016, 11, 1804-1811.	1.6	6
120	Composition of the Essential Oil of Coristospermum cuneifolium and Antimicrobial Activity Evaluation. Planta Medica International Open, 2017, 4, e74-e81.	0.3	6
121	Human estrogen receptor Î± antagonists, part 2: Synthesis driven by rational design, inÂvitro antiproliferative, and inÂvivo anticancer evaluation of innovative coumarin-related antiestrogens as breast cancer suppressants. European Journal of Medicinal Chemistry, 2022, 227, 113869.	2.6	6
122	Foeniculum vulgare Miller, a New Chemotype from Montenegro. Plants, 2022, 11, 42.	1.6	6
123	Synthesis of new disoxaril analogues with potent and selective anti-human rhinovirus 14 activity. Bioorganic and Medicinal Chemistry Letters, 1991, 1, 575-578.	1.0	5
124	Indolyl aryl sulphones as HIV-1 reverse transcriptase inhibitors: docking and 3D QSAR studies. Expert Opinion on Drug Discovery, 2007, 2, 87-114.	2.5	5
125	Gasâ€phase basicity of 2â€furaldehyde. Journal of Mass Spectrometry, 2012, 47, 1488-1494.	0.7	5
126	Breakthroughs in Medicinal Chemistry: New Targets and Mechanisms, New Drugs, New Hopesâ€“5. Molecules, 2019, 24, 2415.	1.7	5

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127	Breakthroughs in Medicinal Chemistry: New Targets and Mechanisms, New Drugs, New Hopesâ€“7. Molecules, 2020, 25, 2968.	1.7	5
128	Human Estrogen Receptor Î± Antagonists. Part 1: 3-D QSAR-Driven Rational Design of Innovative Coumarin-Related Antiestrogens as Breast Cancer Suppressants through Structure-Based and Ligand-Based Studies. Journal of Chemical Information and Modeling, 2021, 61, 5028-5053.	2.5	5
129	Methyl-2-Thienylketopolymethyleneoxyphenyl Derivatives of Alkyl-Substituted 4,5-Dihydro-Oxazoles with Anti-Human Picornavirus Activity. Antiviral Chemistry and Chemotherapy, 1996, 7, 213-220.	0.3	4
130	Breakthroughs in Medicinal Chemistry: New Targets and Mechanisms, New Drugs, New Hopesâ€“4. Molecules, 2019, 24, 130.	1.7	4
131	Variation in essential oil content and composition of Ridolfia segetum Moris based on 30-hour prolonged fractionated extraction procedure. Natural Product Research, 2020, 34, 1923-1926.	1.0	4
132	Gas-phase structures and thermochemical properties of protonated 5-HMF isomers. International Journal of Mass Spectrometry, 2020, 447, 116237.	0.7	4
133	Discovery of the First Human Arylsulfatase A Reversible Inhibitor Impairing Mouse Oocyte Fertilization. ACS Chemical Biology, 2020, 15, 1349-1357.	1.6	4
134	Ligand-based and structure-based studies to develop predictive models for SARS-CoV-2 main protease inhibitors through the 3d-qsar.com portal. Journal of Computer-Aided Molecular Design, 2022, 36, 483-505.	1.3	4
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